Coulomb Gap in the Density of States of Disordered Metals in Two Dimensions

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We calculate the effect of Coulomb interactions on the average density of states $\nu(\omega)$ of two-dimensional disordered electrons. It is shown that for weak disorder the most singular terms in the perturbative expansion of $\nu(\omega)$ can be summed by means of a simple gauge transformation, which also establishes a relation between the low-frequency behavior of $\nu(\omega)$ and the average conductivity $\sigma(\omega)$. Using this relation, we show that if $\lim_{\omega\to 0} \sigma(\omega) < \infty$, then $\nu(\omega) \sim C|\omega|/e^4$ for $\omega\to 0$, where C is a dimensionless constant and e is the charge of the electron. This implies that a normal metallic state of disordered electrons in two dimensions is not a Fermi liquid.

PACS numbers: 71.23.-k, 71.30.+h, 72.15.Rn

In two dimensions arbitrarily weak disorder causes non-interacting electrons to localize, so that the conductivity vanishes in the thermodynamic limit [1]. For many years it was generally accepted that electron-electron interactions do not qualitatively change this scenario. The recent experimental discovery of a metal-insulator transition in two-dimensional (2d) semiconductor devices [2] was therefore a surprise, and showed that the current theoretical understanding of electron-electron interactions in disordered electronic systems is incomplete. The experiment [2] was analyzed in the light of a generalized scaling theory [3], but a microscopic understanding is still lacking. Motivated by these exciting new developments, in this work we shall re-examine the effect of long-range Coulomb interactions on the average density of states (DOS) $\nu(\omega)$ of disordered electrons in two dimensions.

It is well known that Coulomb interactions drastically modify the DOS in the vicinity of the Fermi energy μ . For example, in the strongly localized regime they give rise to a gap in the DOS at the Fermi energy (Coulomb-gap), which in 2d is of the form [4]

$$\nu(\omega) \sim C|\omega|/e^4$$
 , $\omega \to 0$, (1)

where C is a dimensionless coefficient and e is the charge of the electron [5]. On the other hand, for weak disorder (i.e. for $k_F \ell \gg 1$, where k_F is the Fermi wave-vector and ℓ is the elastic mean free path) a perturbative calculation to first order in the dynamically screened Coulomb interaction yields in two dimensions [6],

$$\nu(\omega) \approx \nu_0 \left[1 - \frac{r_0}{4} \ln(|\omega| \tau_1) \ln(|\omega| \tau_0) \right] , \qquad (2)$$

where we have defined

$$r_0 = [(2\pi)^2 \mathcal{D}_0 \nu_0]^{-1} , \quad \tau_1 = \tau_0 [\mathcal{D}_0 \kappa^2 \tau_0]^{-2} .$$
 (3)

Here $\nu_0 = m/2\pi$ is average DOS (per spin) at the Fermi energy of non-interacting electrons with mass m, $\mathcal{D}_0 = v_F \ell/2$ is the classical diffusion coefficient (where v_F is the Fermi velocity), $\tau_0 = \ell/v_F$ is the elastic lifetime, and κ is the Thomas-Fermi screening wave-vector [7]. Note that $r_0 = (\pi k_F \ell)^{-1}$ is a dimensionless measure for the resistance of the system at the frequency scale $\omega \approx \tau_0^{-1}$.

Obviously the correction term in Eq.(2) diverges for $\omega \to 0$, indicating the breakdown of perturbation theory. It is tempting to speculate that at sufficiently small frequencies Eq.(2) should eventually cross over to Eq.(1), at least if the localization length ξ is finite. Because for non-interacting electrons in the weakly localized regime $\xi \propto \exp[1/r_0]$ is exponentially large, the crossover should only be visible at exponentially small frequency scales. Indeed, resummations of the leading logarithms [8–11] in the regime of weak disorder (where $r_0 \ll 1$) indicate that in 2d the DOS vanishes for $\omega \to 0$, but the precise manner in which this happens has not been clarified [11,12].

It is instructive to recall the origin of the \ln^2 -divergence in Eq.(2). The average DOS of an interacting Fermi system can be calculated from the Fourier transform of the retarded Green's function $G_R(\mathbf{r}, \mathbf{r}', t)$,

$$\nu(\omega) = -\frac{1}{\pi} \text{Im} \int_{-\infty}^{\infty} dt e^{i\omega t} \overline{G_R(\mathbf{r}, \mathbf{r}, t)} , \qquad (4)$$

where the overline denotes averaging over the disorder. By translational invariance, the average is independent of the position r. In a perturbative approach, the corrections to the DOS are obtained by expanding G_R in powers of the interaction and averaging each term in the expansion over the disorder, using the impurity diagram technique. The Feynman diagram responsible for the \ln^2 -singularity in Eq.(2) is shown in Fig.1(a). This diagram has the special property that at small wavevectors $(|\mathbf{q}| \ll \ell^{-1})$ and low frequencies $(|\omega| \ll \tau_0^{-1})$ the diffusive motion of the electrons leads to singular corrections to the charge vertices, which in turn strongly enhance the contribution from the long-wavelength and low-energy part of the dynamically screened Coulomb interaction. The vertex corrections involve so-called Diffuson-diagrams (Fig.1(b)), which within the Matsubara formalism renormalize the charge vertices for frequencies in the regime $\tilde{\omega}_n(\tilde{\omega}_n + \omega_m) < 0$ by a singular factor

$$\Lambda(\mathbf{q}, i\omega_m; i\tilde{\omega}_n) = [\tau_0(\mathcal{D}_0\mathbf{q}^2 + |\omega_m|)]^{-1}.$$
 (5)

Here $\tilde{\omega}_n = 2\pi (n + \frac{1}{2})/\beta$ is the fermionic frequency carried by the external Green's functions, and $\omega_m = 2\pi m/\beta$ is

the bosonic frequency carried by the interaction. β is the inverse temperature. Due to these singular vertex corrections, the main contribution to the diagram in Fig.1(a) comes from energy-momentum transfers satisfying

$$|\omega_m|/\mathcal{D}_0\kappa \ll |\mathbf{q}| \ll (|\omega_m|/\mathcal{D}_0)^{1/2} , |\omega_m| \ll \tau_0^{-1} .$$
 (6)

In this regime, the dynamically screened averaged Coulomb interaction is within the random-phase approximation (RPA, see Fig.1(c,d)) given by [6]

$$\overline{f}_{\mathbf{q},i\omega_m}^{\text{RPA}} \approx (2\mathcal{D}_0 \nu_0)^{-1} |\omega_m|/\mathbf{q}^2 \ .$$
 (7)

From Eqs.(4–7) it is now straightforward to show that the exchange diagram in Fig.1(a) indeed gives rise to the \ln^2 -correction in Eq.(2).

For our calculation described below it is crucial that this \ln^2 -correction is entirely due to Coulomb interactions with momentum transfers small compared with k_F . In other words, the singularity is due to forward scattering. Recently non-perturbative methods have been developed [13] to study electron-electron interactions with dominant forward scattering in clean systems. We shall now show that the functional bosonization approach described in Ref. [13](a) can be generalized such that for weak disorder the dominant corrections to the DOS can be summed to all orders in the dynamically screened Coulomb interaction.

We begin with a number of exact manipulations of the real space, imaginary time Green's function $G(\mathbf{r}, \mathbf{r}', \tau - \tau')$ for a given realization of the disorder. Representing G as a Grassmannian functional integral, decoupling the interaction in the particle-hole channel by means of a Hubbard-Stratonovich (HS) field ϕ , and finally integrating over the fermions, we obtain [13](a)

$$G(\mathbf{r}, \mathbf{r}', \tau - \tau') = \frac{\int \mathcal{D}\{\phi\} e^{-S\{\phi\}} \mathcal{G}(\mathbf{r}, \mathbf{r}', \tau, \tau')}{\int \mathcal{D}\{\phi\} e^{-S\{\phi\}}}, \quad (8)$$

where the effective action is given by [14]

$$S\{\phi\} = \frac{\mathcal{V}}{2\beta} \sum_{q} f_{\mathbf{q}}^{-1} \phi_{-q} \phi_{q} - \text{Tr} \ln[1 - \hat{G}_{0} \hat{V}], \qquad (9)$$

and $\mathcal{G}(\mathbf{r}, \mathbf{r}', \tau, \tau')$ satisfies

$$\left[-\partial_{\tau} + \nabla_{\mathbf{r}}^{2}/2m + \mu - V(\mathbf{r}, \tau) - U(\mathbf{r}) \right] \mathcal{G}(\mathbf{r}, \mathbf{r}', \tau, \tau')$$
$$= \delta(\mathbf{r} - \mathbf{r}')\delta^{*}(\tau - \tau') . \quad (10)$$

Here \mathcal{V} is the volume of the system, $f_{\mathbf{q}} = 2\pi e^2/|\mathbf{q}|$ is the Fourier transform of the bare Coulomb interaction in 2d, and \hat{V} and \hat{G}_0 are infinite matrices in momentum-frequency space. The matrix elements of \hat{V} are $[\hat{V}]_{kk'} = i\beta^{-1}\phi_{k-k'}$, and $[\hat{G}_0]_{kk'}$ is the non-interacting Matsubara Green's function for a given realization of the disorder. In Eq.(10) $U(\mathbf{r})$ is the (short-range) disorder potential, $V(\mathbf{r}, \tau) = i\beta^{-1}\sum_{\mathbf{r}}\phi_{\mathbf{r}}$, and $\delta^*(\tau) = \sum_{\mathbf{r}}e^{i\tilde{\omega}_n\tau}$.

 $V(\mathbf{r},\tau) = i\beta^{-1} \sum_{q} \phi_{q}$, and $\delta^{*}(\tau) = \sum_{n} e^{i\tilde{\omega}_{n}\tau}$. Our strategy is now to separate the *dangerous* modes of $V(\mathbf{r},\tau)$ with energy-momentum transfers in the regime (6) (which are responsible for the \ln^2 -singularity in Eq.(2)) from the harmless modes outside this regime. Let us therefore define $V(\mathbf{r},\tau) = V_d(\mathbf{r},\tau) + V_h(\mathbf{r},\tau)$, where $V_d(\mathbf{r},\tau) = i\beta^{-1}\sum_q'\phi_q$, and the prime indicates that the sum is restricted to the regime (6). We then substitute into Eq.(10) the ansatz

$$\mathcal{G}(\mathbf{r}, \mathbf{r}', \tau, \tau') = \mathcal{G}_1(\mathbf{r}, \mathbf{r}', \tau, \tau') e^{\Phi(\mathbf{r}, \tau) - \Phi(\mathbf{r}', \tau')}, \qquad (11)$$

and seek a solution where $\Phi(\mathbf{r}, \tau)$ depends only on the dangerous modes $V_d(\mathbf{r}, \tau)$. It is not difficult to show that one obtains an *exact solution* of Eq.(10) by choosing \mathcal{G}_1 and Φ such that $-\partial_{\tau}\Phi(\mathbf{r}, \tau) = V_d(\mathbf{r}, \tau)$ and [15]

$$\left[-\partial_{\tau} - (-i\nabla_{\mathbf{r}} + \mathbf{A}(\mathbf{r}, \tau))^{2}/2m + \mu - V_{h}(\mathbf{r}, \tau) - U(\mathbf{r}) \right] \times \mathcal{G}_{1}(\mathbf{r}, \mathbf{r}', \tau, \tau') = \delta(\mathbf{r} - \mathbf{r}')\delta^{*}(\tau - \tau'), \quad (12)$$

where $\mathbf{A}(\mathbf{r},\tau) = -i\nabla_{\mathbf{r}}\Phi(\mathbf{r},\tau)$ is a longitudinal vector potential. The equation for $\Phi(\mathbf{r},\tau)$ can be solved trivially, and we obtain for the gauge factor in Eq.(11)

$$e^{\Phi(\mathbf{r},\tau)-\Phi(\mathbf{r}',\tau')} = \exp\left\{\frac{i}{\beta}\sum_{q}'\frac{\phi_{q}}{i\omega_{m}}\left[e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_{m}\tau)}-e^{i(\mathbf{q}\cdot\mathbf{r}'-\omega_{m}\tau')}\right]\right\}. \quad (13)$$

Nested exponentials of this type are familiar from bosonization [13](a). The crucial observation is now that Eq.(13) contains the leading \ln^2 -singularities to all orders in perturbation theory. To see this, note that in Eq.(12) we have succeeded to eliminate from Eq.(10) the dangerous part $V_d(\mathbf{r},\tau)$ of the scalar potential in favour of a longitudinal vector potential. Although the associated current vertices can still be dressed by Diffusons, the vertex corrections are less singular than in the case of density vertices [16]. For example, it is not difficult to check that the diagram analogous to Fig.1(a) with current vertices instead of density vertices does not give rise to any \ln^2 -singularities. From Eq.(11) it is also obvious that the gauge factor $e^{\Phi(\mathbf{r},\tau)-\Phi(\mathbf{r}',\tau')}$ cancels in gauge invariant correlation functions such as the polarization or the conductivity, so that we immediately see that \ln^2 singularities do not appear in the perturbative calculation of these quantities [6,8].

To make further progress, we have to make several approximations, all of which can be systematically improved. (a) First of all, because the fields $\mathbf{A}(\mathbf{r},\tau)$ and $V_h(\mathbf{r},\tau)$ in Eq.(12) do not generate any \ln^2 -singularities in perturbation theory, let us approximate $\mathcal{G}_1(\mathbf{r},\mathbf{r}',\tau,\tau')\approx \mathcal{G}_0(\mathbf{r},\mathbf{r}',\tau-\tau')$. This is sufficient to obtain the leading infrared behavior of the DOS, which is known to be dominated by \ln^2 -singularities [8]. Eq.(8) can then be written as $G(\mathbf{r},\mathbf{r}',\tau)=G_0(\mathbf{r},\mathbf{r}',\tau)e^{Q(\mathbf{r},\mathbf{r}',\tau)}$, where $Q(\mathbf{r},\mathbf{r}',\tau)=\ln\langle e^{\Phi(\mathbf{r},\tau)-\Phi(\mathbf{r}',0)}\rangle$. Here $\langle \ldots \rangle$ denotes averaging over the HS-field as defined in Eq.(8). The Debye-Waller factor $Q(\mathbf{r},\mathbf{r}',\tau)$ can be calculated systematically via a linked cluster expansion in powers of the RPA interaction $f_{\mathbf{qq}',i\omega_m}^{\mathrm{RPA}}$ for a given realization

of the disorder. For the average DOS we only need $Q(0,0,\tau) \equiv Q(\tau)$. (b) We now calculate $Q(\tau)$ in Gaussian approximation, retaining only the first order term in the linked cluster expansion. A simple calculation yields

$$Q(\tau) = -\frac{1}{\beta \mathcal{V}} \sum_{\mathbf{q}\mathbf{q}'\omega_m} \frac{f_{\mathbf{q}\mathbf{q}',i\omega_m}^{\text{RPA}}}{\omega_m^2} [1 - \cos(\omega_m \tau)] . \tag{14}$$

In clean systems with dominant forward scattering the Gaussian approximation can be justified via Wardidentities [13]. In the presence of disorder the situation is not so simple. We shall come back to this problem below, where we shall argue that, at least as long as the system has a finite static conductivity, Eq.(14) leads to qualitatively correct results for $\nu(\omega)$. Note that by integrating over the HS-field before averaging over the disorder we have eliminated the disorder-dependent denominator in Eq.(8). (c) Finally, we approximately average over the disorder, using the factorization $\overline{G(\mathbf{r},\mathbf{r},\tau)} \approx$ $\overline{G_0(\mathbf{r},\mathbf{r},\tau)} \exp[\overline{Q(\tau)}]$. Diagrammatically this amounts to ignoring all terms where impurity lines connect polarization bubbles to other parts of a given Feynman diagram, a standard approximation in the usual diagrammatic approach to weakly disordered electrons [6]. Using Eqs.(3) and (7), we obtain in the limit $\mathcal{V} \to \infty$ and $\beta \to \infty$

$$\overline{Q(\tau)} = \frac{1}{2} \int_0^{\tau_0^{-1}} \frac{d\omega}{\omega} r_0 \ln(\omega/\mathcal{D}_0 \kappa^2) \left[1 - \cos(\omega \tau) \right] . \quad (15)$$

For large τ this implies $\overline{Q(\tau)} \sim -\frac{r_0}{4} \ln(\tau/\tau_1) \ln(\tau/\tau_0)$, where r_0 and τ_1 are defined in Eq.(3). From Eq.(4) we finally obtain after analytic continuation

$$\nu(\omega) \approx \nu_0 \frac{2}{\pi} \int_{\tau_0}^{\infty} dt \frac{\sin(|\omega|t)}{t} \exp\left[-\frac{r_0}{4} \ln(t/\tau_1) \ln(t/\tau_0)\right] . \tag{16}$$

Expanding the right-hand side of Eq.(16) to first order in r_0 , we recover the perturbative result (2), which is valid as long as $-\ln(|\omega|\tau_0) \lesssim \sqrt{1/r_0}$. Keeping in mind that $1/r_0 \gg 1$, we find that there exists an intermediate frequency range $\sqrt{1/r_0} \lesssim -\ln(|\omega|\tau_0) \lesssim 1/r_0$ where Eq.(16) can be approximated by

$$\nu(\omega) \approx \nu_0 \exp\left[-\frac{r_0}{4} \ln(|\omega|\tau_1) \ln(|\omega|\tau_0)\right] , \qquad (17)$$

in agreement with Finkelstein [8]. This is a non-trivial check that the gauge factor (13) indeed contains the dominant singularities. Note that we have derived Eq.(17) without using replicas. For frequencies below the exponentially small scale $\tau_0^{-1} \exp[-1/r_0]$ Eq.(17) is not valid [8,11]. It is easy to show, however, that in this regime Eq.(16) smoothly crosses over to the linear Coulomb gap given in Eq.(1), with the numerical constant $C = 4\pi^{-1/2}\sqrt{r_0}\exp[1/r_0]$. The amazing fact is that for $\omega \to 0$ the prefactor ν_0 in Eq.(16) disappears and is replaced by $|\omega|/e^4$, which in 2d has the same units as ν_0 .

We now argue that if the conductivity $\sigma(\omega)$ does not diverge for $\omega \to 0$, then the true asymptotic low-frequency behavior of the DOS is indeed given by Eq.(1), although our above result for the numerical value of C is not reliable. Let us therefore recall that the parameter r_0 in Eq.(15) is the dimensionless resistance at frequency scale τ_0^{-1} . With the above approximations (b) and (c) we have effectively replaced $S\{\phi\}$ in Eq.(8) by its Gaussian average, which in the regime (6) can be written as

$$\overline{S}\{\phi\} \approx \frac{\mathcal{V}}{\beta(2\pi)^2} \sum_{q} \frac{\mathbf{q}^2}{r_0|\omega_m|} \phi_{-q} \phi_q . \tag{18}$$

In deriving Eq.(15), we have assumed that r_0 is not renormalized for $\omega \to 0$, which is in general incorrect: higher order corrections in the disorder, as well as the non-Gaussian terms neglected in Eq.(18) renormalize the effective value of r_0 at small frequencies, so that in Eq.(18) we should replace $r_0 \to r(i\omega_m)$. Note that $r^{-1}(\omega)$ is proportional to the frequency-dependent conductivity. A microscopic calculation of $r(\omega)$ is beyond the scope of the methods developed in this work. However, we may assume different scenarios for $r(\omega)$ and calculate the consequences for the DOS.

First of all, suppose that $0 < \lim_{\omega \to 0} r(\omega) \equiv r_* < \infty$, so that the system is a normal metal, with a finite static conductivity [17]. In this case the non-Gaussian terms neglected in Eq.(18) are irrelevant (in the renormalization group sense) with respect to the Gaussian fixed point action [18]. We conclude that if interactions stabilize a normal metallic state in 2d [17], then the DOS exhibits a Coulomb gap $\nu(\omega) \sim C|\omega|/e^4$, just like in the strongly localized regime. The numerical value of C depends on r_* , which we have not calculated. Because the DOS vanishes at the Fermi energy, a normal metal in 2d (if it exists) is not a conventional Fermi liquid. Let us emphasize that for our calculation we have assumed that the screening length κ^{-1} is smaller than the mean free path [7]. In contrast, in the strongly localized regime the screening length is infinite and the Coulomb gap can be explained from the classical Hartree energy [4]. Thus, the physics responsible for the Coulomb gap is different in both cases. Numerical evidence that in 2d the Coulomb gap in the DOS survives in a non-Fermi liquid metallic state has been found previously by Efros and Pikus [19].

Depending on the low-frequency behavior of $r(\omega)$, there are two other possibilities. If $r(\omega) \to 0$ for $\omega \to 0$, the system is a perfect metal. This is the physically most plausible scenario, because it is consistent with the generalized scaling theory [3]. In 2d we expect that the divergence of $\sigma(\omega)$ is logarithmic, so that $r(\omega) \sim -\gamma/\ln(\omega\tau_0)$ with $\gamma > 0$. Because the weak logarithmic singularity does not affect the irrelevance of the non-Gaussian terms neglected in Eq.(18), we may calculate $\nu(\omega)$ by substituting $r_0 \to -\gamma/\ln(\omega\tau_0)$ in Eq.(15). This yields $\nu(\omega) \propto |\omega|^{\gamma/2}$. Note that in Ref. [8] Finkelstein found (incorrectly [10,12]) $r(\omega) \sim -\frac{1}{2}/\ln(\omega\tau_0)$. In this case we obtain $\nu(\omega) \propto |\omega|^{1/4}$, in agreement with Ref. [8]. The

third possibility is $r(\omega) \to \infty$ for $\omega \to 0$, so that the system is an *insulator*. Because we know that Eq.(1) is valid for strongly localized electrons [4], and remains correct even if $\sigma(0)$ is finite, by continuity it is extremely plausible that $\nu(\omega) \sim C|\omega|/e^4$ in the entire localized regime.

Experimentally $\nu(\omega)$ can be obtained by measuring the tunneling conductance dI/dV as function of the applied voltage V. Such a measurement was performed in Ref. [20], and the measured dI/dV was compared with the perturbative prediction (2). Keeping in mind that a logarithmic dependence was only observed in a rather small voltage interval, it seems that the data shown in Fig.1 (a) of Ref. [20] are consistent with the emergence of a linear Coulomb gap (1). It would be very interesting to measure the tunneling conductance in the 2d materials that exhibit a metal-insulator transition [2]. On the metallic side of the transition, a linear dependence of dI/dV on the voltage V would be consistent with a finite value of the static conductivity, while a non-linear dependence would be consistent with $\sigma(0) = \infty$.

I would like to thank S. Chakravarty for many discussions and for pressing me to sharpen my arguments. I am also thankful to A. H. Castro-Neto and G. E. Castilla for their hospitality during a visit in Riverside, where part of this work was carried out, and to S. Kivelson for drawing my attention to the work quoted in Ref. [18]. This work was financially supported by the DFG.

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- the back-scattering channel is suppressed. In obtaining this result he used the fact that the conductivity $\sigma(\omega)$ seemed to diverge for $\omega \to 0$. Subsequently a mistake in the renormalization group equations of Ref. [8] was discovered [10], and it was shown that the corrected equations actually imply that $\lim_{\omega \to 0} \sigma(\omega)$ is finite.
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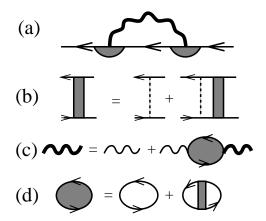


FIG. 1. (a) This exchange correction to the average Green's function gives rise to the \ln^2 -correction to the DOS in Eq.(2). The solid arrows represent non-interacting disorder averaged Green's functions, the shaded semi-circles denote Diffusion corrections defined in (b), and the thick wavy line denotes the dynamically screened interaction defined in (c) and (d). Here the dashed line denotes impurity scattering, and the thin wavy line is the bare interaction.